

# Spectral fluctuations of Schrödinger operators generated by critical points of the potential.

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## Abstract

Starting from the spectrum of Schrödinger operators on  $\mathbb{R}^n$ , we propose a method to detect critical points of the potential. We argue semi-classically on the basis of a mathematically rigorous version of Gutzwiller's trace formula which expresses spectral statistics in term of classical orbits. A critical point of the potential with zero momentum is an equilibrium of the flow and generates certain singularities in the spectrum. Via sharp spectral estimates, this fluctuation indicates the presence of a critical point and allows to reconstruct partially the local shape of the potential. Some generalizations of this approach are also proposed.

keywords : Semi-classical analysis; Schrödinger operators; Equilibriums in classical mechanics.

## 1 Introduction.

### Background.

Let  $P_{\hbar} = -\hbar^2 \Delta + V$  be a Schrödinger operator where the potential  $V$  is smooth on  $\mathbb{R}^n$  and bounded from below. By a standard result in spectral theory,  $P_{\hbar}$  has a unique self-adjoint realization on a dense subset of  $L^2(\mathbb{R}^n)$ . As usually, to this quantum operator  $P_{\hbar}$  we can associate a classical counterpart with the Hamiltonian function  $p(x, \xi) = \xi^2 + V(x)$  on the phase space  $\mathbb{R}^n \times \mathbb{R}^n$ . In what follows, we note  $\Phi_t$  the Hamiltonian flow of  $H_p = \partial_{\xi} p \cdot \partial_x - \partial_x p \cdot \partial_{\xi}$ .

In the present contribution we are particularly interested in a relation between the asymptotic properties of eigenvalues  $\lambda_j(\hbar)$  of  $P_{\hbar}$  :

$$P_{\hbar} \Psi_j(x, \hbar) = \lambda_j(\hbar) \Psi_j(x, \hbar), \quad \hbar \rightarrow 0,$$

and the closed orbits of  $\Phi_t$ . In geometry spectrum and periodic orbits can be related, in a very explicit way, by means of the Selberg and Duistermaat-Guillemin [8] trace formulae. In quantum mechanics, the existence of such a relation is strongly suggested by the correspondence principle which asserts that, in the semiclassical regime  $\hbar \rightarrow 0$ , certain properties of  $P_\hbar$  can be related to  $\Phi_t$ . In the physics literature, a more precise formulation of this principle appeared in the works of Balian&Bloch [1] and Gutzwiller [10]. The Gutzwiller formula is usually stated for the trace of the resolvent :

$$\sum_{j \in \mathbb{N}} \frac{1}{\lambda_j(\hbar) - E} \sim \frac{\text{Vol}(\Sigma_E)}{(2\pi\hbar)^n} + \frac{1}{i\hbar} \sum_{\gamma \in \Sigma_E} A_\gamma e^{\frac{i}{\hbar} S_\gamma}, \quad (1)$$

where in the r.h.s the sum concerns the closed orbits  $\gamma$  inside the surface

$$\Sigma_E = \{(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n / \xi^2 + V(x) = E\}.$$

Also  $\text{Vol}(\Sigma_E)$  is the Riemannian volume of  $\Sigma_E$ ,  $S_\gamma$  and  $A_\gamma$  resp. the classical action and the stability factor, including the Maslov phase, of  $\gamma$ .

In mathematics and in physics, such a relation between spectrum and periodic orbits provides a powerful tool of analysis and computation. See e.g. [14] concerning the asymptotic behavior of eigenvectors  $\Psi_j(x, \hbar)$  and [11] for various applications in quantum chaos. But, for a Schrödinger operator on  $\mathbb{R}^n$ , two different divergences occur in Eq.(1) :

- 1) The sum over the spectrum can be divergent. If the sum is convergent it can also have a divergent behavior when  $\hbar \rightarrow 0$ .
- 2) The sum over closed orbits is generally divergent. This is the case if  $|A_\gamma|$  does not decrease fast enough or if the number of periodic orbits of period smaller than  $T$  is exponentially growing with  $T$ .

#### Mathematical approach of the Gutzwiller formula.

As seen above, the question to remove divergences is important and we explain below how to proceed. Assume that the spectrum of  $P_\hbar$  is discrete in some interval  $[E - \varepsilon, E + \varepsilon]$ , a more global sufficient condition for this is given in section 2. An accessible problem is to study the asymptotic behavior of the spectral distributions :

$$\gamma(E, \hbar, \varphi) = \sum_{|\lambda_j(\hbar) - E| \leq \varepsilon} \varphi\left(\frac{\lambda_j(\hbar) - E}{\hbar}\right), \text{ as } \hbar \rightarrow 0, \quad (2)$$

where  $\varphi$  is a function chosen to remove the divergences. To justify the terminology, observe that the truncated spectral distribution :

$$\sigma_{E, \varepsilon}(x) = \sum_{|\lambda_j(\hbar) - E| \leq \varepsilon} \delta_{\lambda_j(\hbar)}(x),$$

acting on a function  $\varphi$  shifted by  $E$  and scaled w.r.t.  $\hbar$  provides :

$$\gamma(E, \hbar, \varphi) = \left\langle \sigma_{E, \varepsilon}(x), \varphi\left(\frac{x - E}{\hbar}\right) \right\rangle.$$

In general, it is not possible to compute the spectrum of  $P_\hbar$  and one motivation is to derive statistics about eigenvalues. For example, in Eq.(2) the formal choice of  $\varphi$  as the characteristic function of  $[-\eta, \eta]$ ,  $0 < \eta < \varepsilon$ , determines the number  $N(\hbar)$  of bound states in  $[E - \eta\hbar, E + \eta\hbar]$ . Under certain conditions, it can be proven that  $N(\hbar)$  is proportional to  $\hbar^{1-n}$  (Weyl-law). Accordingly, for  $n > 1$  this implies that the finite sum defining  $\gamma(E, \hbar, \varphi)$  involves a large number of eigenvalues as  $\hbar \rightarrow 0$ .

A second aspect is that the asymptotic expansion of  $\gamma(E, \hbar, \varphi)$  involves the classical dynamics in a very explicit way. We recall that  $E$  is regular if  $\nabla p(x, \xi) \neq 0$  on  $\Sigma_E$  and critical otherwise, a critical point  $(x_0, \xi_0)$  of  $p$  is a fixed point of  $\Phi_t$  since  $H_p(x_0, \xi_0) = 0$ . When  $E$  is not critical the asymptotics of Eq.(2) is well determined by the closed orbits of  $\Phi_t$  on  $\Sigma_E$ . For the full treatment of this problem, and a complete formulation of the asymptotic expansion, we refer to [3, 15].

We explain now why the problem stated in Eq.(2) leads to a mathematically rigorous version of the Gutzwiller formula. First, for each  $\hbar > 0$  the sum is finite and a fortiori convergent. A convenient choice of  $\varphi$  also ensures that this quantity has an asymptotic expansion when  $\hbar \rightarrow 0$  independently from the choice of  $\varepsilon$ . On the other side, it will be proven that only the periods of  $\Phi_t$  inside  $\text{supp}(\hat{\varphi})$ , the support of the Fourier transform of  $\varphi$  :

$$\hat{\varphi}(t) = \int_{\mathbb{R}} e^{itx} \varphi(x) dx, \quad (3)$$

contribute in the asymptotic expansion. This principle is useful since when  $\text{supp}(\hat{\varphi})$  is compact then finitely many closed orbits of  $\Sigma_E$  contribute and the second divergence is solved. Hence if  $\hat{\varphi} \in C_0^\infty(\mathbb{R})$ , the space of smooth functions with compact support,  $\varphi$  is in the Schwartz space  $\mathcal{S}(\mathbb{R})$ . Since elements of  $\mathcal{S}(\mathbb{R})$  are smooth with exponential decay at infinity, no divergence occurs and the size of  $\varepsilon$  is irrelevant in the semi-classical approximation.

Finally, in Eq.(2) the scaling w.r.t.  $\hbar$  is important. With this choice and via Fourier transform considerations, we can use the propagator  $U_\hbar(t) = \exp(itP_\hbar/\hbar)$ , solution of the Schrödinger equation :

$$-i\hbar\partial_t U_\hbar(t) = P_\hbar U_\hbar(t),$$

to obtain a precise control w.r.t.  $\hbar$ . Roughly,  $U_\hbar(t)$  can be expanded w.r.t.  $\hbar$  via a so-called WKB approximation. This expansion also provides the explicit relation with the classical dynamics. The precise technical justifications are given in section 3.

### Critical values and contributions of equilibrium.

We have outlined the heuristic relation :

$$\lim_{\hbar \rightarrow 0} \gamma(E, \hbar, \varphi) \rightleftharpoons \{(t, x, \xi) \in \mathbb{R} \times \Sigma_E / \Phi_t(x, \xi) = (x, \xi)\}.$$

In the r.h.s any point  $(x, \xi)$  of a periodic orbit appears only at times  $kT$ ,  $k \in \mathbb{Z}$ , where  $T$  is the primitive period of the orbit. But an equilibrium point  $(x_0, \xi_0)$  satisfies  $\Phi_t(x_0, \xi_0) = (x_0, \xi_0)$  for all  $t$ . Hence when  $E$  is no more a regular value the nature of the set of fixed point changes and some new contributions appear in the asymptotic expansion.

When  $E = E_c$  is critical, the asymptotic behavior of Eq.(2) is more complicated and is closely related to the geometry of the flow inside  $\Sigma_{E_c}$ . For a non-degenerate critical point, i.e.  $d^2p$  is an invertible matrix when  $dp = 0$ , the reader can consult [2]. The problem is treated there for quite general operators, also including the case of a manifold of critical points, but for  $\text{supp}(\hat{\varphi})$  small around the origin. For Schrödinger operators on  $\mathbb{R}^n$  and  $\text{supp}(\hat{\varphi})$  compact but arbitrary, the results of [2] are improved in [13].

Two important problems occur in presence of critical points. First, at every point where  $dp = 0$  the surface  $\Sigma_{E_c}$  and the metric of  $\Sigma_{E_c}$  are not smooth. Next, the determination of the asymptotic expansion w.r.t.  $\hbar$  can be very difficult. The point is that  $\gamma(E, \hbar, \varphi)$  can be expressed in terms of oscillatory integrals :

$$I(\hbar) = \int_{\mathbb{R} \times \mathbb{R}^{2n}} a(t, x, \xi) e^{\frac{i}{\hbar} f(t, x, \xi)} dt dx d\xi, \quad \hbar \rightarrow 0.$$

Note this oscillating factor  $\hbar^{-1}$ , precisely imposed by the scaling w.r.t.  $\hbar$  in Eq.(2). Via the WKB approximation, the phase  $f$  is related to the flow so that the asymptotic behavior of  $I(\hbar)$  is determined by the closed orbits. The technical problem is that, in presence of an equilibrium,  $f$  has some degenerate critical points. The stationary phase method cannot be applied and the asymptotic expansion of  $I(\hbar)$  is radically different : e.g. some terms  $\hbar^\alpha$ ,  $\alpha \in \mathbb{Q}$  and powers of  $\log(\hbar)$  generally appear in this setting.

### Results and strategy.

Our objective is to relate some variations in the discrete spectrum of  $P_\hbar$  with the presence of fixed points for the classical system. Conversely, an attempt is made to prove that the knowledge of such a spectral fluctuation can describe the singularity of the potential. In theory, such a determination is possible since the contributions of equilibria are highly sensitive to the local shape of  $V$ .

We will consider the case of a potential  $V$  with finitely many critical points  $x_0^j$  attached to local homogeneous extremum of  $V$ . An immediate

consequence is that  $p$  admits, locally, a unique critical point  $(x_0^j, 0)$  on the surface  $\Sigma_{E_c^j} = \{(x, \xi) \in \mathbb{R}^{2n} / \xi^2 + V(x) = V(x_0^j)\}$ . A typical example is a polynomial double well in dimension 1 where 3 critical points occur at the 2 minima and at the maximum of  $V$ .

In fact, starting from a more precise relation :

$$\lim_{\hbar \rightarrow 0} \gamma(E, \hbar, \varphi) = \{(t, x, \xi) \in \text{supp}(\hat{\varphi}) \times \Sigma_E / \Phi_t(x, \xi) = (x, \xi)\},$$

the core of the proof lies in 2 facts :

- Equilibriums have a continuous contribution w.r.t. the time  $t$ .
- A convenient choice of  $\text{supp}(\hat{\varphi})$  erases all other contributions.

Here, 'continuous contribution w.r.t.  $t$ ' means that a fixed point contribute to the asymptotic expansion of  $\gamma(E_c^j, \hbar, \varphi)$  in the form  $\hbar^\alpha \log(\hbar)^\beta \langle D, \hat{\varphi} \rangle$  with  $\text{supp}(D) = \mathbb{R}$ . Contrary to standard periodic orbits whom contributions are supported in the set of periods, such a term supported on the line cannot be erased just by shrinking the support of  $\hat{\varphi}$ . For example, if  $\text{supp}(\hat{\varphi})$  contains no period of the flow the analysis easily follows if we view  $\gamma(E, \hbar, \varphi)$  as a function of  $E$  :

- The order w.r.t  $\hbar$  of  $\gamma(E, \hbar, \varphi)$  changes when  $E \rightarrow E_c^j$ . This indicates the presence of an equilibrium for  $\Phi_t$ , a fortiori of a critical point for  $V$ .
- This discontinuity at  $E_c^j$  describes the shape of  $V$ .

## 2 Hypotheses and main result.

Let  $p(x, \xi) = \xi^2 + V(x)$ , where the potential  $V$  is real valued and smooth on  $\mathbb{R}^n$ . To this Hamiltonian is attached the  $\hbar$ -differential operator  $P_\hbar = -\hbar^2 \Delta + V(x)$  and by a classical result  $P_\hbar$  is essentially self-adjoint if  $V$  is bounded from below.

**Remark 1** We are here mainly interested in the case of Schrödinger operators but a generalization to an  $\hbar$ -admissible operator (e.g. in the sense of [17]) of principal symbol  $\xi^2 + V(x)$  is given in the last section.

First, to obtain a well defined spectral problem, we use :

$(H_1)$   $V \in C^\infty(\mathbb{R}^n)$ . *There exists  $C \in \mathbb{R}$  such that  $\liminf_{\infty} V > C$ .*

Note that  $(H_1)$  is always satisfied if  $V$  goes to infinity at infinity. Now, consider an energy interval  $J = [E_1, E_2]$  with  $E_2 < \liminf_{\infty} V$ . In the following we note :

$$J(\varepsilon) = [E_1 - \varepsilon, E_2 + \varepsilon]. \quad (4)$$

For  $\varepsilon < \varepsilon_0$  the set  $p^{-1}(J(\varepsilon))$  is compact. By Theorem 3.13 of [17] the spectrum  $\sigma(P_{\hbar}) \cap J(\varepsilon)$  is discrete and consists in a sequence  $\lambda_1(\hbar) \leq \lambda_2(\hbar) \leq \dots \leq \lambda_j(\hbar)$  of eigenvalues of finite multiplicities, if  $\varepsilon$  and  $\hbar$  are small enough.

The main tool of this work will be the spectral distribution :

$$\gamma(E, \hbar, \varphi) = \sum_{\lambda_j(\hbar) \in J(\varepsilon)} \varphi\left(\frac{\lambda_j(\hbar) - E}{\hbar}\right), \quad (5)$$

more precisely, the asymptotic information contained in this object. To avoid any problem of convergence we impose the condition :

(H<sub>2</sub>) We have  $\hat{\varphi} \in C_0^\infty(\mathbb{R})$  with a sufficiently small support near the origin.

**Remark 2** (H<sub>2</sub>) is used to erase contributions of non-trivial closed orbits and can be relaxed to  $\hat{\varphi} \in C_0^\infty(\mathbb{R})$  with a weaker result. A more precise description of  $\text{supp}(\hat{\varphi})$  is given in Lemma 10. For a non-degenerate minimum, it is more comfortable to assume that  $\text{supp}(\hat{\varphi})$  contains no period of  $d\Phi_t(z_0)$ . Some singularities, not relevant here, are generated by these periods and we refer to [2, 13] for a detailed study of these contributions.

To simplify notations we write  $z = (x, \xi) \in \mathbb{R}^{2n}$  and  $\Sigma_E = p^{-1}(\{E\})$  and we use the subscript  $E_c$  to distinguish out critical values of  $p$ . Of course one can also work with  $T^*\mathbb{R}^n \simeq \mathbb{R}^n \times \mathbb{R}^n$ . In  $J$  there is finitely many critical values  $E_c^1, \dots, E_c^l$  and in  $p^{-1}(J)$  finitely many fixed points  $z_0^1, \dots, z_0^m$ ,  $m \geq l$ . We impose now the type of singularity :

(H<sub>3</sub>) On each  $\Sigma_{E_c^j}$  the symbol  $p$  has isolated critical points  $z_0^j = (x_0^j, 0)$ . These critical points can be degenerate but are associated to a local extremum of  $V$  :

$$V(x) = E_c + V_{2k}(x) + \mathcal{O}(\|x - x_0^j\|^{2k+1}), \quad k \in \mathbb{N}^*, \quad (6)$$

where  $V_{2k}$ , homogeneous of degree  $2k$ , is definite positive or negative.

**Remark 3** For non-degenerate singularities we can apply the results of [2] and the extremum condition is not really necessary.

The next assumption, erases the mean values in the trace formula :

(H<sub>4</sub>)  $\hat{\varphi}$  is flat at 0, i.e.  $\hat{\varphi}^{(j)}(0) = 0$ ,  $\forall j \in \mathbb{N}$ .

We could weaken (H<sub>4</sub>) to  $\hat{\varphi}^{(j)}(0) = 0$ ,  $\forall j \leq j_0$ , where  $j_0$  depends only on the degree of the singularities of  $V$  (cf. section 4). Note that such a  $\varphi$  exists. Pick  $g \in C_0^\infty(\mathbb{R})$ ,  $\text{supp}(g) \subset [-M, M]$ , then  $\hat{\varphi}(t) = t^{2j_0}g(t)$  satisfies our hypotheses. In this case, we can pick  $g$  even so that  $\varphi$  is real.

Finally, to relax a bit  $(H_2)$  we need a control on the contribution of closed orbits. To do so, we impose the classical condition :

$(H_5)$  *All periodic trajectories of the flow are non-degenerate.*

Non-degenerate closed orbits are those whose Poincaré map does not admit 1 as eigenvalue and are isolated. The main result is :

**Theorem 4** Assume  $(H_1)$  to  $(H_4)$  satisfied. As  $\hbar$  tends to  $0^+$ , we have :

$$\gamma(s, \hbar, \varphi) = \begin{cases} \mathcal{O}(\hbar^\infty) & \text{if } s \in [E_1, E_2] \setminus \{E_c^1, \dots, E_c^l\}, \\ \mathcal{O}(f_j(\hbar)) & \text{if } s = E_c^j, j \in \{1, \dots, l\}, \end{cases}$$

where each  $f_j(\hbar)$  has a finite order w.r.t.  $\hbar$ .

Precisely, if  $s = E_c^j$  carries a single minimum of degree  $2k$  we obtain :

$$f_j(\hbar) = C(n, k, \varphi) \hbar^{\frac{n}{2} + \frac{n}{2k} - n}. \quad (7)$$

But for a local maximum of  $V$  we can obtain a logarithm of  $h$  :

$$f_j(\hbar) = C(n, k, \varphi) \hbar^{\frac{n}{2} + \frac{n}{2k} - n} \log(\hbar)^j, \quad j = 0 \text{ or } 1. \quad (8)$$

In fact if the critical surface carries more than one critical point then  $f_j$  is the sum of their respective contributions. Note that for  $n = 1$  and  $k > 1$  the singular term has negative order w.r.t.  $\hbar$ . A more detailed formulation of each  $f_j(\hbar)$  is given in Propositions 12,13. An interesting property is that the singularity of  $\gamma(s, \hbar, \varphi)$  describes partially the singularity of  $V$ .

**Corollary 5** Assume that  $\Sigma_{E_c}$  carries exactly one singularity  $(x_0, 0)$ . Then the discontinuity of  $\gamma(s, \hbar, \varphi)$  at  $s = E_c$  determines the degree of the critical point and the spherical average of the germ of  $V$  in  $x_0$ .

This principle is limited in presence of multiple equilibriums on the same surface since the sum of contributions of each critical point could lead to a compensation. In  $(H_2)$  the condition that  $\text{supp}(\hat{\varphi})$  is small implies a very accurate spectral estimate (e.g. by a Paley-Wiener estimates for  $\varphi$ ). It is possible to relax this assumption but the result is weaker :

**Corollary 6** Assume  $(H_1)$ ,  $(H_3)$ ,  $(H_4)$  and  $(H_5)$  satisfied and that  $\hat{\varphi} \in C_0^\infty(\mathbb{R})$ , then we obtain :

$$\gamma(s, \hbar, \varphi) = \mathcal{O}(1) \text{ if } s \in [E_1, E_2] \setminus \{E_c^1, \dots, E_c^l\}.$$

For critical values of  $p$ , estimates are the same as in Theorem 4.

The justification, given in section 4, is that in this case the asymptotics is given by a finite sum over periodic orbits of energy  $s$ . This result is weak if the singularity of  $V$  is non-degenerate since the equilibrium has a contribution of degree 0 w.r.t.  $\hbar$ . (cf. Propositions 12,13 or section 3 of [2]). Finally, we would like to emphasize that a maximum is more difficult to detect contrary to a local minimum which is isolated on the energy surface.

### 3 Oscillatory representation.

The construction below is more or less classical and will be sketchy. The only change is the choice of a more global localization around  $J = [E_1, E_2]$ . Strictly speaking, with  $(H_1)$ , we could also consider  $] - \infty, E_2]$ . Let be  $\varphi \in \mathcal{S}(\mathbb{R})$  with  $\hat{\varphi} \in C_0^\infty(\mathbb{R})$ , we recall that :

$$\gamma(E, \hbar, \varphi) = \sum_{\lambda_j(\hbar) \in J(\varepsilon)} \varphi\left(\frac{\lambda_j(\hbar) - E}{\hbar}\right), \quad J(\varepsilon) = [E_1 - \varepsilon, E_2 + \varepsilon],$$

with  $p^{-1}(J(\varepsilon))$  compact in  $T^*\mathbb{R}^n$ . For  $\varepsilon > 0$  small enough, we localize around  $J$  with a cut-off  $\Theta \in C_0^\infty(]E_1 - \varepsilon, E_2 + \varepsilon[)$ , such that  $\Theta = 1$  on  $J$  and  $0 \leq \Theta \leq 1$  on  $\mathbb{R}$ . We accordingly split-up our spectral distribution as :

$$\gamma(E, \hbar, \varphi) = \gamma_1(E, \hbar, \varphi) + \gamma_2(E, \hbar, \varphi),$$

with :

$$\begin{aligned} \gamma_1(E, \hbar, \varphi) &= \sum_{\lambda_j(\hbar) \in J(\varepsilon)} (1 - \Theta)(\lambda_j(\hbar)) \varphi\left(\frac{\lambda_j(\hbar) - E}{\hbar}\right), \\ \gamma_2(E, \hbar, \varphi) &= \sum_{\lambda_j(\hbar) \in J(\varepsilon)} \Theta(\lambda_j(\hbar)) \varphi\left(\frac{\lambda_j(\hbar) - E}{\hbar}\right). \end{aligned}$$

Since  $\varphi \in \mathcal{S}(\mathbb{R})$  a classical estimate, see e.g. Lemma 1 of [4], is :

$$\gamma_1(E, \hbar, \varphi) = \mathcal{O}(\hbar^\infty), \quad \text{as } \hbar \rightarrow 0^+. \quad (9)$$

By inversion of the Fourier transform we have :

$$\Theta(P_\hbar) \varphi\left(\frac{P_\hbar - E}{\hbar}\right) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\frac{tE}{\hbar}} \hat{\varphi}(t) \exp\left(-\frac{it}{\hbar} P_\hbar\right) \Theta(P_\hbar) dt.$$

The trace of the left hand-side is  $\gamma_2(E, \hbar, \varphi)$  and Eq.(9) provides :

$$\gamma(E, \hbar, \varphi) = \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} e^{i\frac{tE}{\hbar}} \hat{\varphi}(t) \exp\left(-\frac{it}{\hbar} P_\hbar\right) \Theta(P_\hbar) dt + \mathcal{O}(\hbar^\infty). \quad (10)$$

Eq.(10) is very close to the classical Poisson summation formula on  $\mathbb{S}^1$  since the r.h.s. is expressed below in term of the classical dynamics and this asymptotic relation justifies the terminology of 'trace formula'. Moreover, this formulation shows that the scaling w.r.t.  $\hbar$ , imposed in the definition of  $\gamma(E, \hbar, \varphi)$ , is the best one since we will solve the semi-classical propagator homogeneously w.r.t.  $\hbar$ .

Let  $U_\hbar(t) = \exp(-\frac{it}{\hbar}P_\hbar)$  be the quantum propagator. We approximate  $U_\hbar(t)\Theta(P_\hbar)$  by a Fourier integral operator (FIO) depending on  $\hbar$ . Let  $\Lambda$  be the Lagrangian manifold associated to the flow of  $p$  :

$$\Lambda = \{(t, \tau, x, \xi, y, \eta) \in T^*\mathbb{R} \times T^*\mathbb{R}^n \times T^*\mathbb{R}^n : \tau = p(x, \xi), (x, \xi) = \Phi_t(y, \eta)\},$$

and  $I(\mathbb{R}^{2n+1}, \Lambda)$  the class of oscillatory integrals based on  $\mathbb{R}^{2n+1}$  and whose Lagrangian manifold is  $\Lambda$ . The next result is a semi-classical version of a well known result on the propagator, see e.g. Duistermaat [7].

**Theorem 7** The operator  $U_\hbar(t)\Theta(P_\hbar)$  is an  $\hbar$ -FIO associated to  $\Lambda$ . For each  $N \in \mathbb{N}$  there exists  $U_{\Theta, \hbar}^{(N)}(t)$  with integral kernel in Hörmander's class  $I(\mathbb{R}^{2n+1}, \Lambda)$  and  $R_\hbar^{(N)}(t)$  bounded, with a  $L^2$ -norm uniformly bounded for  $0 < \hbar \leq 1$  and  $t$  in a compact subset of  $\mathbb{R}$ , such that :

$$U_\hbar(t)\Theta(P_\hbar) = U_{\Theta, \hbar}^{(N)}(t) + \hbar^N R_\hbar^{(N)}(t).$$

This result provides the existence of an asymptotic expansion in power of  $\hbar$  with a remainder that can be controlled since  $\text{supp}(\hat{\varphi})$  is a compact. After perhaps a reduction of  $\varepsilon$ , this remainder  $R_\hbar^{(N)}(t)$  is estimated via :

**Corollary 8** Let  $\Theta_1 \in C_0^\infty(\mathbb{R})$ , with  $\Theta_1 = 1$  on  $\text{supp}(\Theta)$  and  $\text{supp}(\Theta_1) \subset ]E_1 - 2\varepsilon, E_2 + 2\varepsilon[$ , then  $\forall N \in \mathbb{N}$  :

$$\text{Tr}(\Theta(P_\hbar)\varphi(\frac{P_\hbar - E}{\hbar})) = \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} \hat{\varphi}(t) e^{\frac{i}{\hbar}tE} U_{\Theta, \hbar}^{(N)}(t) \Theta_1(P_\hbar) dt + \mathcal{O}(\hbar^{N-n}).$$

For a proof of this result, based on the cyclicity of the trace and a priori estimates on the spectral projectors (see [17]), we refer to [4]. For the particular case of a Schrödinger operator the BKW ansatz shows that the integral kernel of  $U_{\Theta, \hbar}^{(N)}(t)$  can be recursively constructed as :

$$K_\hbar^{(N)}(t, x, y) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} b_\hbar^{(N)}(t, x, y, \xi) e^{\frac{i}{\hbar}(S(t, x, \xi) - \langle y, \xi \rangle)} d\xi,$$

$$b_\hbar^{(N)} = b_0 + \hbar b_1 + \dots + \hbar^N b_N,$$

where  $S$  satisfies the Hamilton-Jacobi equation :

$$p(x, \partial_x S(t, x, \xi)) + \partial_t S(t, x, \xi) = 0,$$

with initial condition  $S(0, x, \xi) = \langle x, \xi \rangle$ . In particular we obtain that :

$$\{(t, \partial_t S(t, x, \eta), x, \partial_x S(t, x, \eta), \partial_\eta S(t, x, \eta), -\eta)\} \subset \Lambda,$$

and that the function  $S$  is a generating function of the flow, i.e. :

$$\Phi_t(\partial_\eta S(t, x, \eta), \eta) = (x, \partial_x S(t, x, \eta)). \quad (11)$$

We insert this approximation in Eq.(10), we set  $x = y$  and we integrate w.r.t.  $x$ . Modulo an error  $\mathcal{O}(\hbar^{N-n})$ , we obtain that  $\gamma(E, \hbar, \varphi)$  equals :

$$\frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R} \times T^*\mathbb{R}^n} e^{\frac{i}{\hbar}(S(t, x, \xi) - \langle x, \xi \rangle + tE)} a_\hbar^{(N)}(t, x, \xi) \hat{\varphi}(t) dt dx d\xi, \quad (12)$$

where  $a_\hbar^{(N)}(t, x, \eta) = b_\hbar^{(N)}(t, x, x, \eta)$ .

**Remark 9** By Theorem 3.11 & Remark 3.14 of [17],  $\Theta(P_\hbar)$  is  $\hbar$ -admissible. Moreover, the symbol is compactly supported in  $p^{-1}([E_1 - \varepsilon, E_2 + \varepsilon])$ . This point allows to consider only oscillatory integrals with compact support for the evaluation of the spectral distributions.  $\square$

#### Microlocalization of the trace.

If  $\psi \in C_0^\infty(T^*\mathbb{R}^n)$ , we recall that  $\psi^w(x, \hbar D_x)$  is the linear operator obtained by Weyl-quantization of  $\psi$ , i.e. :

$$\psi^w(x, \hbar D_x) f(x) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar}\langle x-y, \xi \rangle} \psi\left(\frac{x+y}{2}, \xi\right) f(y) dy d\xi.$$

Mainly, the contribution of an equilibrium  $z_0 \in \Sigma_{E_c}$  can be reached via :

$$\gamma_{z_0}(E_c, \hbar, \varphi) = \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} e^{i\frac{tE_c}{\hbar}} \hat{\varphi}(t) \psi^w(x, \hbar D_x) \exp(-\frac{i}{\hbar} t P_\hbar) \Theta(P_\hbar) dt, \quad (13)$$

where  $\psi \in C_0^\infty(T^*\mathbb{R}^n)$  is equal to 1 near  $z_0$ . This principle will also be useful to obtain a weak generalization in presence of multiple equilibriums.

We recall some basics on symbolic calculus with FIO. Hörmander's class of distributions with Lagrangian manifold  $\Lambda$  over  $\mathbb{R}^n$  is noted  $I(\mathbb{R}^n, \Lambda)$ . If  $(x_0, \xi_0) \in \Lambda$  and  $\varphi(x, \theta) \in C^\infty(\mathbb{R}^n \times \mathbb{R}^N)$  parameterizes  $\Lambda$  in a sufficiently small neighborhood  $U$  of  $(x_0, \xi_0)$ , then for each  $u_\hbar \in I(\mathbb{R}^n, \Lambda)$  and  $\chi \in$

$C_0^\infty(T^*\mathbb{R}^n)$ ,  $\text{supp}(\chi) \subset U$ , there exists a sequence of amplitudes  $c_j(x, \theta) \in C_0^\infty(\mathbb{R}^n \times \mathbb{R}^N)$  such that for all  $L \in \mathbb{N}$  :

$$\chi^w(x, \hbar D_x) u_\hbar = \sum_{-d \leq j < L} \hbar^j I(c_j e^{\frac{i}{\hbar} \varphi}) + \mathcal{O}(\hbar^L).$$

Hence, for each  $N \in \mathbb{N}^*$  and modulo an error  $\mathcal{O}(\hbar^{N-d})$ , the localized trace  $\gamma_{z_0}(E_c, \hbar, \varphi)$  of Eq.(13) can be written as :

$$(2\pi\hbar)^{-d} \int_{\mathbb{R} \times \mathbb{R}^{2n}} e^{\frac{i}{\hbar}(S(t,x,\xi) - \langle x, \xi \rangle + tE_c)} \tilde{a}_\hbar^{(N)}(t, x, \xi) \hat{\varphi}(t) dt dx d\xi. \quad (14)$$

To get the right power  $-d$  of  $\hbar$ , we apply results of Duistermaat [7] on the order :  $\hbar$ -pseudo-differential operators  $\psi^w(x, \hbar D_x)$  are of order 0 w.r.t.  $1/\hbar$ . Since the order of  $U_\hbar(t)\Theta(P_\hbar)$  is  $-\frac{1}{4}$ , we have :

$$\psi^w(x, \hbar D_x) U_\hbar(t) \Theta(P_\hbar) \sim (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} \tilde{a}_\hbar^{(N)}(t, x, y, \eta) e^{\frac{i}{\hbar}(S(t,x,\eta) - \langle y, \eta \rangle)} dy.$$

Multiplying by  $\hat{\varphi}(t) e^{\frac{i}{\hbar} t E_c}$  and passing to the trace we find Eq.(14) with  $d = n$  and we write again  $\tilde{a}_\hbar^{(N)}(t, x, \eta)$  for  $\tilde{a}_\hbar^{(N)}(t, x, x, \eta)$ . In particular :

$$\tilde{a}_\hbar^{(0)}(t, x, x, \eta) = \psi(x, \eta) a_0(t, x, x, \eta), \quad (15)$$

is independent of  $\hbar$  and is compactly supported w.r.t.  $(x, \eta)$ .

## 4 Proof of the main result.

### Classical dynamics near the equilibrium.

A generic critical points of the phase function of Eq.(12) satisfies :

$$\begin{cases} E = -\partial_t S(t, x, \xi), \\ x = \partial_\xi S(t, x, \xi), \\ \xi = \partial_x S(t, x, \xi), \end{cases} \Leftrightarrow \begin{cases} p(x, \xi) = E, \\ \Phi_t(x, \xi) = (x, \xi), \end{cases}$$

where the right hand side defines a closed trajectory of the flow inside  $\Sigma_E$ . Note that equilibriums are also included. By the non-stationary phase lemma, outside of the critical set the contribution is  $\mathcal{O}(\hbar^\infty)$ .

Let be  $E_c$  any critical value in  $[E_1, E_2]$  and  $z_0$  an equilibrium of  $\Sigma_{E_c}$ . We choose a function  $\psi \in C_0^\infty(T^*\mathbb{R}^n)$ , with  $\psi = 1$  near  $z_0$ , hence :

$$\begin{aligned} \gamma_2(E_c, \hbar, \varphi) &= \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} e^{i \frac{t E_c}{\hbar}} \hat{\varphi}(t) \psi^w(x, \hbar D_x) \exp(-\frac{i}{\hbar} t P_\hbar) \Theta(P_\hbar) dt \\ &+ \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} e^{i \frac{t E_c}{\hbar}} \hat{\varphi}(t) (1 - \psi^w(x, \hbar D_x)) \exp(-\frac{i}{\hbar} t P_\hbar) \Theta(P_\hbar) dt. \end{aligned}$$

If there is no other singularity on  $\Sigma_{E_c}$  with  $(H_5)$  the asymptotic expansion of the second term is given by the semi-classical trace formula on a regular level. For finitely many critical point on  $\Sigma_{E_c}$ , we can repeat the procedure. The first term is micro-local and precisely generate the singularity in Theorem 4. We note  $\Omega$  the discrete set of critical points  $z_0^j$  in  $p^{-1}(J)$ . The next result provides a global information on the periods of the classical flow.

**Lemma 10** There exists a  $T > 0$ , depending only on  $V$  and  $J = [E_1, E_2]$ , such that  $\Phi_t(z) \neq z$  for all  $z \in p^{-1}(J) \setminus \Omega$  and all  $t \in ]-T, 0[ \cup ]0, T[$ .

*Proof.* If  $H_p$  is our hamiltonian vector field and  $z = (x, \xi)$  we have :

$$\|H_p(z_1) - H_p(z_2)\|^2 = 4\|\xi_1 - \xi_2\|^2 + \|\nabla_x V(x_1) - \nabla_x V(x_2)\|^2.$$

When  $z_1$  and  $z_2$  are in the compact  $p^{-1}(J)$  there exists  $b > 0$  such that :

$$\|\nabla_x V(x_1) - \nabla_x V(x_2)\| \leq b\|x_1 - x_2\|.$$

Hence, there exists  $a > 0$  such that :

$$\|H_p(z_1) - H_p(z_2)\| \leq a\|z_1 - z_2\|, \quad \forall z_1, z_2 \in p^{-1}(J).$$

The main result of [18] shows that any periodic orbit inside  $p^{-1}(J)$  has a period  $\tau \geq 2\pi/a > 0$ . The lemma follows with  $T := T(V, J) = 2\pi/a$ . ■

**Remark 11** The result of [18] is optimal (harmonic oscillator). Note that  $T$  is decreasing if one increase the size of  $J$ . Lemma 10 provides a total control on the r.h.s. of the trace formula : if  $\hat{\varphi} \in C_0^\infty(]-T, T[)$ , the only contribution arises from the set  $\{(t, z_0), t \in \text{supp}(\hat{\varphi})\}$ .

Now, we restrict our attention to the singular contribution generated by one critical point. As pointed out in section 2, for a non degenerate extremum a minor technical problem could occur. We recall that the linearized flow  $d\Phi_t$  is the differential of the flow  $\Phi_t$  w.r.t. initial conditions  $z = (x, \xi)$ . When  $z_0$  is a critical point of  $p$ , the linear map  $z \mapsto d\Phi_t(z_0)z$  can be interpreted as the Hamiltonian flow of  $z \mapsto \langle d^2p(z_0)z, z \rangle$ . After perhaps a change of local coordinates near  $x_0$ , we can assume that  $d^2V(x_0)$  is diagonal. If  $x_0$  is a maximum of the potential  $d\Phi_t(z_0)$  has no non-zero period which ends immediately the discussion. If  $x_0$  is a minimum  $d\Phi_t(z_0)$  is elliptic with primitive periods  $(T_1, \dots, T_n)$  generated by the eigenvalues of  $d^2V(x_0)$ . But the constant  $b$  of Lemma 10 is certainly bigger than the spectral radius of  $d^2V(x_0)$  and hence we have the inequality  $T < \min\{T_1, \dots, T_n\}$ . Following the approach of [2] or [13], if  $\text{supp}(\hat{\varphi}) \subset ]-T, T[$  the associated contribution is smooth on  $\text{supp}(\hat{\varphi}) \setminus \{0\}$ . For a degenerate critical point as in  $(H_3)$  a surprising result, established in [5, 6], is that the only singularity is located

at  $t = 0$ . Hence no extra assumption on  $\hat{\varphi}$  is required.

**The trace as an energy function.**

As seen in section 2 it suffices to study the localized problem :

$$\gamma_{z_0}(E_c, \hbar, \varphi) = \frac{1}{2\pi} \text{Tr} \int_{\mathbb{R}} e^{i \frac{t E_c}{\hbar}} \hat{\varphi}(t) \psi^w(x, \hbar D_x) \exp(-\frac{it}{\hbar} P_h) \Theta(P_h) dt.$$

Here  $\psi \in C_0^\infty(T^*\mathbb{R}^n)$  is micro-locally supported near  $z_0$  (cf section 2). For the convenience of the reader we recall the contributions of equilibria in the trace formula. We note  $S(\mathbb{S}^{n-1})$  the surface of  $\mathbb{S}^{n-1}$  and in the next two propositions it is understood that conditions  $(H_1)$  to  $(H_3)$  are satisfied.

**Proposition 12** If  $x_0$  is a local minimum we have :

$$\gamma_{z_0}(E_c, \hbar, \varphi) \sim \hbar^{\frac{n}{2} + \frac{n}{2k} - n} \sum_{j, l \in \mathbb{N}^2} \hbar^{\frac{j}{2} + \frac{l}{2k}} \Lambda_{j, l}(\varphi),$$

where the  $\Lambda_{j, l}$  are some distributions. The leading coefficient is :

$$\hbar^{\frac{n}{2} + \frac{n}{2k} - n} \frac{S(\mathbb{S}^{n-1})}{(2\pi)^n} \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-\frac{n}{2k}} d\eta \int_{\mathbb{R}_+ \times \mathbb{R}_+} \varphi(u^2 + v^{2k}) u^{n-1} v^{n-1} dudv.$$

**Proposition 13** If  $x_0$  is a local maximum we have :

$$\gamma_{z_0}(E_c, \hbar, \varphi) \sim \hbar^{\frac{n}{2} + \frac{n}{2k} - n} \sum_{m=0,1} \sum_{j, l \in \mathbb{N}^2} \hbar^{\frac{j}{2} + \frac{l}{2k}} \log(\hbar)^m \Lambda_{j, l, m}(\varphi).$$

If  $\frac{n(k+1)}{2k} \notin \mathbb{N}$ , the first non-zero coefficient is given by :

$$\hbar^{\frac{n}{2} + \frac{n}{2k} - n} \langle T_{n, k}, \varphi \rangle \frac{S(\mathbb{S}^{n-1})}{(2\pi)^n} \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-\frac{n}{2k}} d\eta.$$

The distributions  $T_{n, k}$  are respectively given by :

$$\begin{aligned} \langle T_{n, k}, \varphi \rangle &= \int_{\mathbb{R}} (C_{n, k}^+ |t|_+^{\frac{n(k+1)}{2k} - 1} + C_{n, k}^- |t|_-^{\frac{n(k+1)}{2k} - 1}) \varphi(t) dt, \text{ if } n \text{ is odd,} \\ \langle T_{n, k}, \varphi \rangle &= C_{n, k}^- \int_{\mathbb{R}} |t|_-^{\frac{n(k+1)}{2k} - 1} \varphi(t) dt, \text{ if } n \text{ is even.} \end{aligned}$$

But if  $\frac{n(k+1)}{2k} \in \mathbb{N}$  and  $n$  is odd then the top-order term is :

$$C_{n, k} \log(\hbar) \hbar^{\frac{n}{2} + \frac{n}{2k} - n} \frac{S(\mathbb{S}^{n-1})}{(2\pi)^n} \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-\frac{n}{2k}} d\eta \int_{\mathbb{R}} |t|^{\frac{n(k+1)}{2k} - 1} \varphi(t) dt.$$

Finally, if  $\frac{n(k+1)}{2k} \in \mathbb{N}$  and  $n$  is even,  $C_{n,k}^+ = C_{n,k}^-$  and we have :

$$C_{n,k}^\pm \hbar^{\frac{n}{2} + \frac{n}{2k} - n} \frac{1}{(2\pi)^n} \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-\frac{n}{2k}} d\eta \int_{\mathbb{R}} |t|^{n\frac{k+1}{2k}-1} \varphi(t) dt.$$

**Remark 14** To emphasize the consistency of these results we precise that  $C_{n,k}$ ,  $C_{n,k}^\pm$  are non-zero universal constants depending only on  $n$  and  $k$ . Such terms  $\hbar^\alpha$  and  $\hbar^\alpha \log(\hbar)$ ,  $\alpha \in \mathbb{Q}$  never appear if  $E$  is regular.

For a proof we refer to [5, 6] resp. for a local minimum and maximum. The case  $k = 1$  was treated in [2]. With  $(H_5)$  and  $E$  regular, we have :

$$\begin{aligned} \gamma(E, \hbar, \varphi) &\sim \frac{\hbar^{1-n}}{(2\pi)^n} \text{LVol}(\Sigma_E) \hat{\varphi}(0) + \sum_{j=1}^{\infty} \hbar^{1-n+j} c_j(\hat{\varphi})(0) \\ &+ \sum_{\rho \in \Sigma_E} e^{\frac{i}{\hbar} S_\rho} e^{i\pi\mu_\rho/4} \sum_{j=0}^{\infty} D_{\rho,j}(\hat{\varphi})(T_\rho) \hbar^j. \end{aligned}$$

We refer to [15] for a proof. In the r.h.s. the sum concerns periodic orbits  $\rho$  of energy  $E$  and is finite since  $\text{supp}(\hat{\varphi})$  is compact. Here  $S_\rho$ ,  $\mu_\rho$  and  $T_\rho$  are resp. the action, the Maslov-index and the period of the closed orbit  $\rho$  and both  $c_j$ ,  $D_{\rho,j}$  are differential operators of order  $j$ . If  $\varphi$  satisfies  $(H_4)$  we have  $c_j(\hat{\varphi})(0) = 0$  and for each  $s \in [E_1, E_2]$  regular :

$$\gamma(s, \hbar, \varphi) \sim \sum_{\rho \in \Sigma_s} e^{\frac{i}{\hbar} S_\rho} e^{i\pi\mu_\rho/4} \sum_{j=0}^{\infty} D_{\rho,j}(\hat{\varphi})(T_\rho) \hbar^j. \quad (16)$$

We accordingly obtain that :

$$\gamma(s, \hbar, \varphi) = \mathcal{O}(1), \quad \forall s \in [E_1, E_2] \setminus \{E_c^1, \dots, E_c^l\}. \quad (17)$$

This point will justify Corollary 6. By Lemma 10, we have  $T_\rho \geq T$  uniformly w.r.t.  $s \in [E_1, E_2]$ . Hence if  $s$  is not critical and  $(H_2)$  is satisfied the sum over the periods of Eq.(16) is simply 0 and in Eq.(17) we obtain in fact  $\mathcal{O}(\hbar^\infty)$ . Note that  $(H_5)$  is not required here. For  $s = E_c^m$  critical there is a continuous contribution w.r.t.  $t$  in the spectral distribution. A fortiori, a choice of  $\hat{\varphi}$  flat at the origin does not erase this term. We have :

$$\gamma(E_c^m, \hbar, \varphi) \sim \sum_{j=1}^{N_m} f_j(\hbar),$$

where  $N_m$  is the number of equilibrium on  $\Sigma_{E_c^m}$  and each  $f_j(\hbar)$  is given by the leading term of Propositions 12,13. ■

Note that the bottom of a symmetric double well gives a similar answer as a single well of same nature. Hence without microlocal considerations it is difficult to distinguish these 2 different settings.

*Proof of corollary 5.* First, the Weyl-law for regular energies :

$$\gamma(E, \hbar, \varphi) \sim (2\pi\hbar)^{1-n} \hat{\varphi}(0) \text{Lvol}(\Sigma_E),$$

computes the dimension  $n$ . Now assume given a critical value  $E_c$  with a single critical point. The only choice of the spectral function  $\varphi$  allows to detect  $E_c$  via the singularity  $f(\hbar)$  of Theorem 4. The knowledge of  $f(\hbar)$  determines the order of the contribution. For example, if :

$$f(\hbar) \sim C\hbar^\alpha \log(\hbar),$$

the critical point is a maximum and  $\alpha$  computes the degree  $2k$  of the singularity. With  $\hat{\varphi}$ , the knowledge of  $k$  allows to compute the quantity :

$$\int_{\mathbb{R}} |t|^{n\frac{k+1}{2k}-1} \varphi(t) dt.$$

A fortiori  $C$  determines the average of  $|V_{2k}|^{-\frac{n}{2k}}$  on  $\mathbb{S}^{n-1}$ . Without  $\log(\hbar)$ , the nature of the critical point can be detected by a symmetry argument w.r.t.  $\varphi$  since we a priori know  $n$  and  $k$ . In view of Propositions 12,13 we can choose  $\varphi$  odd, even, symmetric or non-symmetric w.r.t. the origin to conclude. Note that if  $\hat{\varphi}$  is not even  $\varphi$  is a priori complex valued. ■

The spherical average of  $V_{2k}$  is a Jacobian. For example we have :

$$\int_{\mathbb{R}^n} e^{-|V_{2k}(x)|} dx = \frac{1}{2k} \Gamma\left(\frac{n}{2k}\right) \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-\frac{n}{2k}} d\eta.$$

A similar result holds for the pullback  $f(V_{2k}(x))$ , if  $f \in L^1(\mathbb{R}_+, r^{\frac{n}{2k}-1} dr)$ .

**Remark 15** Enlarging the list of singularities would provide a bigger "dictionary". The case of non-homogeneous singularities for  $V$  is still an open problem, in particular because the determination of an explicit asymptotic expansion w.r.t.  $\hbar$  can be very difficult.

We propose now 2 slight generalizations of the main result.

**a) Effect of a sub-principal symbol.**

Because of some recent developments of Helffer&Sjöstrand for Witten Laplacians, see e.g. [12] for an overview and references, we show shortly how to

extend the result of Theorem 4 to the case of an  $\hbar$ -admissible operator. For example, the Witten Laplacian on zero-forms is :

$$\Delta_{f,\hbar}^{(0)} = -\hbar^2 \Delta + \frac{1}{4} |\nabla f(x)|^2 - \frac{\hbar}{2} \Delta f(x), \quad f \in C^\infty(\mathbb{R}^n),$$

whose symbol  $p(x, \xi) = p_0(x, \xi) + \hbar p_1(x, \xi)$  depends on  $\hbar$ . More generally, it is possible to consider operators  $P_\hbar$  of symbol  $p_\hbar \sim \sum \hbar^j p_j$  (Borel sum) with principal symbol  $p_0(x, \xi) = \xi^2 + V(x)$  and a subprincipal symbol  $p_1 \neq 0$ . Starting from the results of section 3 we proceed as follows.

To each element  $u_\hbar$  of  $I(\mathbb{R}^n, \Lambda)$  we can associate canonically a principal symbol  $e^{\frac{i}{\hbar} S} \sigma_{\text{princ}}(u_\hbar)$ , where  $S$  is a function on  $\Lambda$  such that  $\xi dx = dS$  on  $\Lambda$ . In fact, if  $u_\hbar$  can locally be represented by an oscillatory integral with amplitude  $a$  and phase  $\varphi$ , then we have  $S = S_\varphi = \varphi \circ i_\varphi^{-1}$  and  $\sigma_{\text{princ}}(u_\hbar)$  is a section of  $|\Lambda|^{\frac{1}{2}} \otimes M(\Lambda)$ , where  $M(\Lambda)$  is the Maslov vector-bundle of  $\Lambda$  and  $|\Lambda|^{\frac{1}{2}}$  the bundle of half-densities on  $\Lambda$ . When  $p_1 \neq 0$ , in the global coordinates  $(t, y, \eta)$  on  $\Lambda$ , the half-density of  $U_\hbar(t)$  is given by :

$$\nu(t, y, \eta) = \exp(i \int_0^t p_1(\Phi_s(y, -\eta)) ds) |dt dy d\eta|^{\frac{1}{2}}. \quad (18)$$

For this expression, related to the resolution of the first transport equation for the propagator, we refer to Duistermaat and Hörmander [9]. Accordingly, the FIO approximating the propagator has the amplitude :

$$\tilde{a}(t, z) = a(t, z) \exp(i \int_0^t p_1(\Phi_s(z)) ds).$$

Since  $z_0$  is an equilibrium we have  $p_1(\Phi_s(z_0)) = p_1(z_0)$ ,  $\forall s$ , and :

$$\tilde{a}(t, z_0) = \hat{\varphi}(t) e^{it p_1(z_0)}. \quad (19)$$

If the subprincipal symbol vanishes at the critical point, which is the case in a lot of practical situations, the trace formula remains the same. If  $p_1(z_0) \neq 0$ , by Fourier inversion formula we replace  $\varphi(t)$  by  $\varphi(t + p_1(z_0))$  in all integral formulae of Propositions 12,13. Note that, with  $(H_4)$ , this has absolutely no effect for the mean values and hence on the main result.

#### b) A micro-local approach.

We inspect now the case of an energy surface supporting more than one critical point, but with a much more restrictive method. Let be  $K = p^{-1}(J) \subset T^*\mathbb{R}^n$  and  $r_0 = \frac{1}{2} \inf_{i \neq j} d(z_i, z_j)$ , where  $d$  is any distance on  $T^*\mathbb{R}^n$ . Each open ball  $B(z, r_0) \subset T^*\mathbb{R}^n$  contains at most 1 critical point for each  $z \in K$ .

Clearly, we can cover a compact neighborhood of  $K$  by a finite number of balls  $B(z, r_0)$ . With a partition of unity, adapted to this covering, we obtain :

$$\sum_{j=1}^N \psi_j^w(x, \hbar D_x) = \text{Id, on } C_0^\infty(K).$$

For each  $s \in J$ , we obtain :

$$\text{Tr} \int_{\mathbb{R}} \hat{\varphi}(t) \Theta(P_{\hbar}) e^{\frac{i}{\hbar} t(P_{\hbar} - s)} dt = \sum_{j=1}^N \text{Tr} \int_{\mathbb{R}} \hat{\varphi}(t) \psi_j^w(x, \hbar D_x) \Theta(P_{\hbar}) e^{\frac{i}{\hbar} t(P_{\hbar} - s)} dt.$$

Note that the r.h.s. is studied in section 2. By the same argument as before, if  $\Sigma_s \cap \text{supp}(\psi_j)$  contains no critical point we obtain :

$$\text{Tr} \int_{\mathbb{R}} \hat{\varphi}(t) \psi_j^w(x, \hbar D_x) \Theta(P_{\hbar}) e^{\frac{i}{\hbar} t(P_{\hbar} - s)} dt = \mathcal{O}(\hbar^\infty).$$

And if there is exactly one critical point  $z_0 \in \Sigma_s$  in  $\text{supp}(\psi_j)$  we have :

$$\text{Tr} \int_{\mathbb{R}} \hat{\varphi}(t) \psi_j^w(x, \hbar D_x) \Theta(P_{\hbar}) e^{\frac{i}{\hbar} t(P_{\hbar} - s)} dt = \psi(z_0) f_j(\hbar),$$

and by construction no cancellation can occur.

**Remark 16** In Corollary 6 we have considered  $(H_5)$  for the flow. A similar result holds for a chaotic dynamics and an isolated degenerate closed orbit can be treated as in [16]. Finally, using the results of [15] one can extend Corollary 6 to the case of families of periodic orbits of dimension  $d \leq n$ .

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